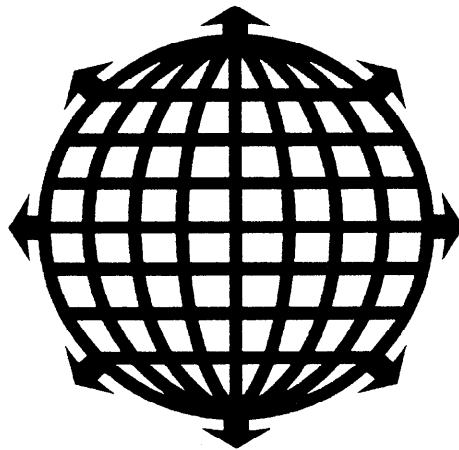


MAY 6 - 1997

GOLDEN, COLORADO 80401-3393

**PROCEEDINGS OF**  
**SOLAR '96**  
**THE 1996**  
**AMERICAN SOLAR ENERGY SOCIETY**  
**ANNUAL CONFERENCE**

**Asheville, North Carolina**  
**April 13-18, 1996**



**Editors:**  
**R. Campbell-Howe**  
**B. Wilkins-Crowder**

**American Solar Energy Society**  
**2400 Central Avenue, Suite G-1**  
**Boulder, Colorado 80301**

*Printed on recycled paper*

# **SOLSCALE: SOFTWARE TO PREDICT SCALING IN SOLAR DOMESTIC HOT WATER SYSTEMS**

**Derek Baker**

**Gary Vliet**

**Desmond Lawler**

**College of Engineering**

**The University of Texas at Austin, Austin, Texas 78712**

## **ABSTRACT**

The software SOLSCALE was developed to predict calcium carbonate scaling in solar domestic hot water (SDHW) systems. It requires inputs of make-up water chemistry, system design specifications, water demand, and location. Scaling predictions are based on an equilibrium water chemistry model and a system operating temperature model. The equilibrium water chemistry model accounts for ion activities, calcium complexes, and temperature dependencies in the equilibrium constants. Operating temperatures are interpolated from a database of representative values based on the location's weather, and the nondimensional variables SA/L (insolation x collector area / energy load) and V/Q (storage volume / daily load volume). The severity of scaling is predicted and recommendations are made to alleviate the problem when appropriate. SOLSCALE is available on 3 1/2" disks for PCs with Windows Version 3.1 or later.

## **1. INTRODUCTION**

Deterioration of the performance of SDHW systems due to scale formation has been documented in areas with hard water (1,2,3). Scaling is primarily the result of calcium carbonate precipitating out of water onto a surface. Due to calcium carbonate's decreasing solubility with increasing temperature for almost all water types, it normally occurs on the heat transfer surfaces where the potable water reaches its maximum temperature. The scaled surface's higher heat transfer resistance results in decreased system efficiency. The presence of severe scale can also adversely affect system reliability, an example being possible freeze

damage in drain-back systems. The software SOLSCALE was developed to predict scaling so that appropriate actions could be taken to alleviate the problem during a SDHW system's design phase.

Scaling is primarily a function of a water's chemistry and temperature. Traditionally, the Langelier Index has been used to predict scaling by industry personnel and has proved to be fairly reliable in predicting if a water will scale, but not as reliable in predicting the amount a water will scale. An equilibrium-water-chemistry scaling model was developed by Loewenthal and Marais (4) and adopted for research into SDHW system scaling first by Singh, Cheng, and Chopra (2) and then by Burch, Egrikan, and Carlisle (1). The current research expands on this equilibrium-water-chemistry model and links it with a SDHW system operating temperature model to form SOLSCALE. Details on this research are contained in a report to the National Renewable Energy Laboratory by Vliet, Lawler, and Baker (5). SOLSCALE is intended for use by SDHW industry personnel to predict scaling.

## **2. WATER CHEMISTRY**

### **2.1. Equilibrium Model**

The water chemistry model is based on the principles of equilibrium chemistry, which assume that there is an infinite amount of time for the water to reach equilibrium conditions. In SDHW systems this represents a worst case scenario, because it assumes that all of the water's possible scale will form on the heat transfer surfaces, called herein the water's *potential scaling*. Actual scaling should be

less than the potential scaling, because for low levels of oversaturation some scaling will probably occur downstream from the heat transfer surfaces, and additionally, water can remain slightly oversaturated indefinitely. The equilibrium chemistry model provides an initial quantitative indication of scaling.

The inputs for the model are the water's analysis temperature, pH, total alkalinity, dissolved calcium, and either its total dissolved solids or specific conductance. Based on these inputs the model iterates to find the equilibrium values of pH, total alkalinity, and dissolved calcium that would result in the water being in equilibrium with solid calcium carbonate for temperatures between 0 and 100°C. Subtracting the equilibrium calcium concentration from the inputted value gives the amount of calcium per liter of water that must precipitate as calcium carbonate in order for the water to reach equilibrium. This model includes corrections for ion activities, calcium complex concentrations (dissolved  $\text{CaCO}_3^0$ ,  $\text{CaOH}^+$ , and  $\text{CaHCO}_3^+$ ), and temperature dependencies in the equilibrium constants. The most significant change in equilibrium conditions with temperature is the decreasing solubility of calcium carbonate with increasing temperature, which causes the worst scaling to occur on heat transfer surfaces.

## 2.2. Degree of Oversaturation and Scaling Fraction

The rate of scale formation is related to a water's degree of oversaturation with calcium carbonate. All other things being equal, the greater a water is oversaturated with calcium carbonate, the greater the rate of scale formation. A scaling rate approximation is included in the equilibrium model by calculating the water's degree of oversaturation and introducing a scaling fraction, multiplier that estimates the portion of the potential scale that will actually form based on the water's degree of oversaturation.

Equilibrium calcium carbonate precipitation, or scaling, is controlled by the equation

$$K'_{so} = [\text{Ca}^{2+}] [\text{CO}_3^{2-}] \quad (1)$$

where  $K'_{so}$  is the equilibrium constant modified to account for activity coefficients, and  $[\text{Ca}^{2+}]$  and  $[\text{CO}_3^{2-}]$  are the equilibrium calcium ion and carbonate ion concentrations in the water. For a water oversaturated with calcium carbonate,  $\text{CaCO}_3$ , equilibrium chemistry predicts that calcium carbonate will precipitate until this equation is satisfied. A water's degree of oversaturation

(DOS) has been defined as the number of times  $K'_{so}$  has been exceeded, i.e.,

$$\text{DOS} = \frac{[\text{Ca}^{2+}]_{IN} [\text{CO}_3^{2-}]_{IN}}{K'_{so}} \quad (2)$$

where  $[\text{Ca}^{2+}]_{IN}$  and  $[\text{CO}_3^{2-}]_{IN}$  are the inputted calcium ion and carbonate ion concentrations in the water. Precipitation can occur when  $\text{DOS} > 1$ . Because it is known that the precipitation that forms scale will not always occur to the extent predicted by equilibrium, the calcium carbonate in excess of equilibrium conditions is classified into three groups according to the water's DOS, and a different portion of the potential scale ( $S^P$ ) is assumed to form from each. The three categories are defined as follows:

- (1)  $S^P_{1-3}$ : The dissolved calcium carbonate in excess of the equilibrium condition (1 times oversaturated) but less than the 3 times oversaturated condition;
- (2)  $S^P_{3-8}$ : The dissolved calcium carbonate in excess of the 3 times oversaturated condition, but less than the 8 times oversaturated condition;
- (3)  $S^P_{8+}$ : The dissolved calcium carbonate in excess of the 8 times oversaturated condition.

The model is run three times, once to calculate the dissolved calcium carbonate in excess of true equilibrium conditions and twice to calculate the dissolved calcium carbonate in excess of the 3 and 8 times oversaturated conditions. Because water can dissolve calcium carbonate scale if it is undersaturated, a negative contribution to calcium carbonate scale formation is allowed. From these three runs the potential scaling from each DOS range, e.g.  $S^P_{1-3}$ , can be calculated by subtraction. A water undersaturated with dissolved calcium carbonate would have a  $S^P_{1-3} < 0$ ,  $S^P_{3-8} = 0$ , and  $S^P_{8+} = 0$ , while a water greatly oversaturated with dissolved calcium carbonate would have all  $S^P$  values greater than zero.

It is assumed that scaling more readily occurs with increasing DOS; that is, the fraction of the potential scale to form will increase with increase in DOS. The fractions of potential scale that are predicted to form, called scaling fractions (SF), are estimated to be 0.2, 0.6, and 1.0 for the moderate, high, and very high degrees of oversaturation, respectively. Multiplying the scaling fractions by the potential calcium carbonate scale associated with each degree of oversaturation and summing gives the total *predicted scale*. The selection of the oversaturation levels 1, 3, and 8 was based on estimates from the literature of

critical oversaturation levels (6, 7) and can be easily modified if warranted by new information and experience.

### **3. MAXIMUM DAILY OPERATING TEMPERATURE MODEL**

Due to the large dependency of scaling on water temperature, it was necessary to develop a model to estimate the maximum-daily-operating-temperatures (MDOT) that the potable water would reach in a SDHW system. Experience has shown that most severe scaling occurs where the potable water reaches its maximum temperature, which is in the collector for direct systems and the heat exchanger for indirect systems (1, 3). Because most SDHW systems in the US are indirect systems, it was decided to base the MDOT model on water temperatures inside the heat exchanger and not the collector.

The MDOT model is based on a database of simulations performed for representative SDHW systems located in different parts of the United States using TRNSYS, a SDHW simulation program (8). MDOT histograms were developed for 23 weather categories in the United States, and the histograms indicate the number of days per year that the system's MDOTs are in 5°C bins over the range 0 to 100°C. The model requires the following five inputs:

- (1) Location: The city in the database of 212 US cities closest to the location of interest.
- (2) Collector Area: The area of the solar collector.
- (3) Storage Volume: The entire tank volume for single-tank systems and the solar tank volume for dual-tank systems.
- (4) Total Daily Hot Water Demand: The volume of the daily hot water demand.
- (5) Average Make-Up Water Temperature: The average annual temperature of the make-up water to the system. A default value is available based on the city chosen, assuming a surface water supply.

Based on this information, the model interpolates among 69 MDOT histograms from the database (three histograms for each of the 23 weather categories) to develop a final histogram.

Three variables are needed to interpolate MDOT histograms from the database: (1) SA/L (annual horizontal insolation x collector area / annual energy load), (2) V/Q (storage volume / daily hot water volume demand), and, (3) the location's weather as classified into one of twenty-three categories. Interpolation is based on two

correlations. The first is that within the same weather category, similar MDOT histograms exist for systems with the same values of SA/L and V/Q. The second is that within the same weather category, similar MDOT histograms can also exist for different combinations of SA/L and V/Q, and functional relationships have been developed to relate these values of SA/L and V/Q.

The twenty-three weather categories were defined using monthly average-daily weather data for 212 US cities. The categories were based on the following four weather parameters: (1) total annual insolation on a surface tilted at latitude plus 10° (tilted insolation), (2) the maximum divided by the minimum monthly average-daily tilted insolation, (3) average annual ambient temperature, and (4) the maximum minus the minimum monthly average-daily ambient temperature.

Representative annual MDOT histograms were generated for each weather category using a typical single-tank indirect system using TRNSYS. Nine representative histograms were created for each weather category, based on systems with low, medium, and high operating temperatures, 50, 80, and 120 gallon storage tank volumes, and an 80 gallon per day hot water load. Figure 1 shows the nine MDOT histograms for weather category 23. The systems were sized such that the three histograms (50, 80, and 120 gallon storage) in each operating temperature range (low, medium, and high) were similar. For each weather category a best-fit exponential equation was then found that related the three SA/L and V/Q values at each operating temperature. Figure 2 shows the exponential relations developed for weather category 23. The 80 gallon storage tank cases were used as the nominal histograms for each operating temperature range and are saved in the database.

### **4. COMBINING THE EQUILIBRIUM CHEMISTRY AND MDOT MODELS**

The dynamics of a SDHW system are complex and can change drastically from one system to the next, especially with respect to the amount and timing of the hot water load. The MDOT simulations in TRNSYS used a slightly modified RAND hot water demand profile (9) with peak hot water demands occurring in the morning and evening but with some demand occurring throughout the day. A simplifying assumption is made in predicting scaling by assuming that the scaling is essentially a batch process. This effectively means that there is no hot water demand while a SDHW system is heating the water. The water's supply chemistry is the inputted water chemistry and the

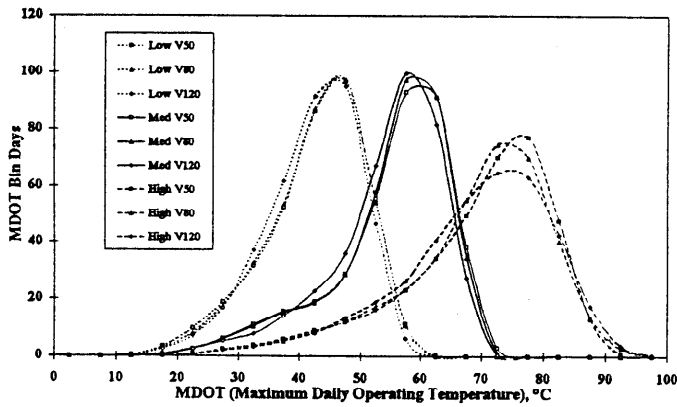


Fig. 1 Annual Histogram of Maximum Daily Operating Temperature. Low, Med, and High refer to the operating temperature range, and V50, V80, and V120 refer to a 50, 80, and 120 gallon storage tank, respectively.

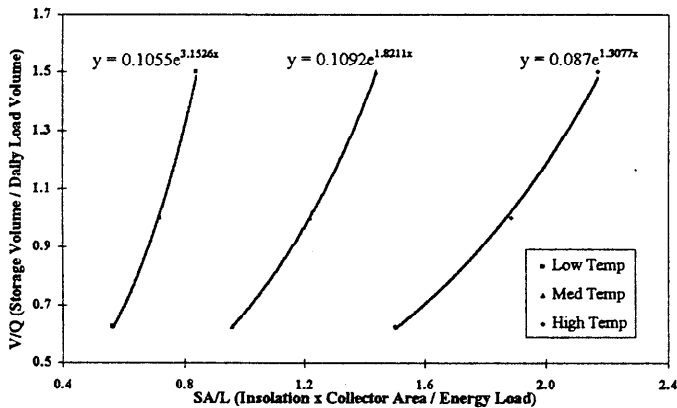


Fig. 2 V/Q versus SA/L, where Low, Med, and High Temp refer to the operating temperature range.

entire batch of water is assumed to reach the system's MDOT. SOLSCALE calculates the *annual scale* (mass of scale / unit area of collector) to form in the heat exchanger as follows:

$$S_A = \frac{1}{A_C} \sum_{DOS=1-3,3-8,8+} \left\{ \sum_{T=2.5}^{97.5} [SF_{DOS} \times S_{DOS,T}^P \times BD_T \times DV] \right\} \quad (3)$$

The terms are defined as follows:

**S<sub>A</sub>:** Predicted Annual Scale, the total mass of calcium carbonate per unit area of collector that may form each year.

**SF and DOS:** The "Scaling Fraction" and "Degree of Oversaturation", respectively. When calculating the

predicted annual scale, SF is equal to 0.2, 0.6, and 1.0 when DOS is in the range of 1-3, 3-8, and greater than 8, respectively.

**T:** The water temperature, which has values between 2.5 and 97.5°C, in 5°C increments.

**S<sup>P</sup>:** Potential scale per volume of water at a given DOS and T, as defined in section 2.2.

**BD:** Bin Days, the number of days in a year the SDHW system's maximum-daily-operating-temperature (MDOT) is in a 5°C bin with average temperature T.

**DV:** Daily Volume, the amount of fresh make-up water introduced into the system each day. If the storage volume exceeds the daily hot-water demand volume, this is assumed to equal the daily hot-water demand volume. If the storage volume is less than the daily hot-water demand volume, this is assumed to equal the storage volume.

**A<sub>C</sub>:** Collector Area. The total scaling is divided by the collector area to provide both a measure of the scale thickness and a comparison of predicted scaling rates between different sized systems. Although the model is based on an indirect system (scaling in the heat exchanger), the scaling per unit of collector area is calculated because the exchanger area is often not readily known. The heat exchanger area is usually approximately proportional to the collector area.

## 5. RECOMMENDATIONS BASED ON THE PREDICTED SCALING

Based on the predicted scaling, one or more of the following six recommendations are given to the user:

- (1) Based on this model, scaling is not predicted to be a problem.
- (2) If the system is not already indirect, such a system is recommended, with the potable water running through the inner tube and the collector fluid in the annulus of the heat exchanger. Routing the potable water through the inner tube will allow for easy inspection and removal of any scale that may occur.
- (3) Check the system after two years for scaling.
- (4) If feasible, try increasing the storage size and/or decreasing the collector size. This can reduce the scaling problem for certain (but not all) types of water. Rerun this program and follow the new recommendations.

- (5) Clean potable water side of the heat exchanger every two years to remove any scale. Possible cleaning methods include routing with a wire brush or the circulation of a 1:10 diluted solution of muriatic acid until the scale is removed.
- (6) Use a water conditioner/softener system. Determine the water quality resulting from conditioning / softening, and rerun this program to confirm that water conditioning/softening will alleviate the scaling problem. Follow the new recommendations.

SOLSCALE classifies the severity of scaling into one of four categories based on the predicted annual scale and offers the following recommendations as numbered above, where the predicted annual scale is in grams  $\text{CaCO}_3$  per square foot of collector per year:

**No Problem:** Predicted Annual Scale  $\leq 0.5$

Recommendation: (1)

**Moderate Problem:**  $0.5 < \text{Predicted Annual Scale} \leq 2$

Recommended Minimum Steps: (2), (3)

Recommended Possible Design Modifications: (4)

**Large Problem:**  $2 < \text{Predicted Annual Scale} \leq 10$

Recommended Minimum Steps: (2), (5)

Recommended Possible Design Modifications: (4), (6)

**Extreme Problem:** Predicted Annual Scale  $> 10$

Recommended Minimum Steps: (2), (6)

Recommended Possible Design Modifications: (3)

## 6. USING SOLSCALE

SOLSCALE is written in Visual Basic and requires Windows Version 3.1 or later to operate. It includes help screens to aid the user in understanding the software. Units can be changed between English (ppm,  $^{\circ}\text{F}$ ,  $\text{ft}^2$ , and gallons) and metric (mg/l,  $^{\circ}\text{C}$ ,  $\text{m}^2$ , and liters) for the water chemistry and system information inputs. Initially the user enters the system's location (state and city), make-up water chemistry, system design information, and hot water demand on the *Input* screen and then chooses the *Run* key to analyze the inputs. Figure 3 shows a sample SOLSCALE *Input* screen for a system located in El Paso, Texas.

After the software calculates the system's potential and predicted scaling, the *Conclusions* screen is displayed giving the annual scale predicted, the classification of the scaling problem, and recommendations to alleviate scaling. Figure 4 shows a sample SOLSCALE *Conclusions* screen based on the inputs in Figure 3. At this point in SOLSCALE, all of the critical information has been given to the user. The user can obtain more detailed information by calling an *Output Details* screen, which displays the potential and predicted scaling occurring at each level of oversaturation and the water's Langelier Index at three critical temperatures. Three graphs are also available to the user:

- (1) Water Scaling Potential versus Temperature: The milligrams of  $\text{CaCO}_3$  that have the potential to form

### Inputs:

Location:		State: <input type="text" value="Texas"/>	Choose a State
		City: <input type="text" value="El Paso"/>	Choose a City
<b>Water Chemistry Data:</b>		*Metric Units were chosen for the Water Chemistry Data	
Water Analysis Temperature:	<input type="text" value="25.0"/> $^{\circ}\text{C}$ (25 $^{\circ}\text{C}$ Default)	Total Alkalinity:	<input type="text" value="142.0"/> mg/l as $\text{CaCO}_3$
pH:	<input type="text" value="8.0"/>	Dissolved Calcium:	<input type="text" value="45.0"/> mg/l as Calcium
Total Dissolved Solids (TDS), mg/l		<input type="text" value="556.0"/>	
Specific Conductance, $\mu\text{mho/cm}$		<input type="text" value="556.0"/>	
<b>SDHW System Information:</b>		*English Units were chosen for the SDHW System Information	
Collector Area:	<input type="text" value="40.0"/> $\text{ft}^2$	<input type="button" value="Run"/> <input type="button" value="Cancel"/> <input type="button" value="Quit"/> <input type="button" value="Help"/>	
Storage Volume:	<input type="text" value="80.0"/> gallons		
Total Daily Hot Water Load:	<input type="text" value="80.0"/> gallons (Nominal load is 20 gallons/person/day)		
Avg Make-up Water Temp:	<input type="text" value="61.5"/> $^{\circ}\text{F}$ (Default value based on location)		

Fig. 3 SOLSCALE Input Screen

### Conclusions:

**Annual Scale Predicted:** 7.1 grams of  $\text{CaCO}_3$  per  $\text{ft}^2$  of Collector

Based on the amount of predicted scaling, there is a LARGE SCALING PROBLEM predicted. This agrees very well with the Langelier Index at the weighted average temperature of 62.5 $^{\circ}\text{C}$ .

### Recommendations:

#### Minimum Steps:

- If the system is not already indirect, such a system is recommended, with the potable water running through the inner tube and the collector fluid in the annulus of the heat exchanger. Routing the potable water through the inner tube will allow for easy inspection and removal of any scale that may occur.
- Clean potable water side of the heat exchanger every two years to remove any scale. Possible cleaning methods include routing with a wire brush or the circulation of a 1:10 diluted solution of muriatic acid until the scale is removed.

#### Possible Design Modifications:

- If feasible, try increasing the storage size and/or decreasing the collector size. This can reduce the scaling problem for certain (but not all) types of water. Rerun this program and follow the new recommendations.
- Use a water conditioner/softener system. Determine the water quality resulting from conditioning/softening, and rerun this program to confirm that water conditioning/softening will alleviate the scaling problem. Follow the new recommendations.

<input type="button" value="Change Inputs"/>
<input type="button" value="Output Details"/>
<input type="button" value="Quit"/>
<input type="button" value="Help"/>

Fig. 4 SOLSCALE Conclusions Screen

- from one liter of water at each temperature bin classified according to its degree of oversaturation.
- (2) Histogram of the System's Maximum Daily Operating Temperatures: An annual histogram of the number of days the system's MDOT is within each temperature bin.
- (3) System's Scaling Potential versus Temperature: The grams of  $\text{CaCO}_3$  per square foot of collector that has the potential to form ( $\text{SF} = 1$ ) in each temperature bin classified according to its degree of oversaturation.

## **7. FUTURE WORK**

Currently a kinetic water chemistry model is being developed that includes reaction and ion diffusion rates to predict a water's scaling rate. This model will be integrated into SOLSCALE as another measure of predicting the degree of scaling in a SDHW system. SOLSCALE is still in the developmental phase and needs to be field tested to determine its effectiveness in quantifying scaling in terms of its affect on performance. Due to budgetary constraints, it is not presently known if such field testing will be performed in the near future.

## **8. ACKNOWLEDGMENTS**

This work is being funded by the U.S. Department of Energy (through the National Renewable Energy Laboratory) under contract DE-FG36-94 G010034.

## **9. REFERENCES**

- (1) Burch, J., N. Egrican, N. Carlisle, Calcium Carbonate Scaling in Solar Domestic Hot Water Systems, Proceedings of the 1990 Annual Conference, American Solar Energy Society, Austin, TX, March 1990
- (2) Singh, T., C.F. Cheng, P.S. Chopra, Prediction of Calcium Carbonate Scaling from Water in Solar-Energy Systems, ANL/SDP-TM-79-7, Argonne National Laboratory, IL, 1979
- (3) Vliet, G., Design of Solar Hot Water Systems for Scale Prevention/Remediation, Proceedings of Solar Engineering 1992, ASME/JSES/KSES International Solar Energy Conference, Vol. 1 Pages 201-206, Maui, HI, April 1992

(4) Loewenthal, R.E., G.V.R. Marais, Carbonate Chemistry of Aquatic Systems, Ann Arbor Science Publishers: Ann Arbor, MI, 1976

(5) Vliet, G, D. Lawler, D. Baker, Software to Predict Scaling in Solar Domestic Hot Water Systems, DE-FG36-94 G010034, Report to National Renewable Energy Laboratory, CO, Nov. 1995

(6) Lawler, D., Personal conversation and notes from his class and upcoming book on water quality and treatment, Department of Civil Engineering, University of Texas at Austin, September - November, 1994

(7) Ferguson, R.J., A Kinetic Model for Calcium Carbonate Deposition, Materials Performance, vol. 23, pp. 25-34, 1984

(8) University of Wisconsin at Madison, Solar Energy Laboratory, TRNSYS: A Transient System Simulation Program Users Manual, Madison, WI, 1990

(9) Farrington, R.B., L.M. Murphy, D.L. Noreen, A Comparison of Six Generic Solar Domestic Hot Water Systems, ERI/RR-351-413, Solar Energy Research Institute, CO, 1980